Electrons scattering in the monolayer graphene with the short-range impurities

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Scattering problem for electrons in monolayer graphene with short-range perturbations of the types "local chemical potential" and "local gap" has been solved. Zero gap and non-zero gap kinds of graphene are considered. The determined S-matrix can be used for calculation of such observables as conductance and optical absorption.

During the last years much attention was payed to the problem of the electronic spectrum of graphene (see a review [1]). Two-dimensional structure of it and a presence of the cone points in the electronic spectrum make actual a comprehensive study of the external fields effect on the spectrum and other characteristics of the electronic states described by the Dirac equation in the 2+1 space-time. We consider in this work the electrons scattering in the 2+1 Dirac equation model of the monolayer graphene due to the short-range perturbations. We do not take into account the inter-valley transitions. Particular attention to this case stems from the effectiveness of short-range scatterers in contrast to the long-range ones: an effect of the latter is suppressed by the Klein paradox [2]. Short-range potential impurities in graphene were considered in works [3], [4], [5]. In our work [6], a new model of the short-range impurities in graphene was considered taking into account the obvious fact that the Kohn-Luttinger matrix elements of the short-range perturbation calculated on the upper and lower band wave functions are not equal in a general case. This means that the perturbation must be generically described by a Hermitian matrix. We considered the diagonal matrix case corresponding to a presence of the potential and mass perturbation. The bound states dependence on the perturbation parameters was studied in [6] within the framework of this model.

In the present work we study the electrons scattering by the short-range impurities within the framework of the model suggested in [6].

The Dirac equation describing electronic states in graphene reads

$$\left(-i\hbar v_F \sum_{\mu=1}^{2} \gamma_\mu \partial_\mu - \gamma_0 \left(m + \delta m\right) v_F^2\right) \psi = \left(E - V\right) \psi, \tag{1}$$

where v_F is the Fermi velocity of the band electrons, γ_μ are the Dirac matrices

$$\gamma_0 = \sigma_3,\ \gamma_1 = \sigma_1,\ \gamma_2 = i\sigma_2,$$

σ_i are the Pauli matrices, $2m{v_F}^2 = E_g$ is the electronic bandgap, $\psi\left(\mathbf{r}\right)$ is the two-component spinor. The electronic gap can appear in the graphene monatomic film lying on the substrate because of the sublattices mutual shift [7]. The spinor structure takes into account the two-sublattice structure of graphene. $\delta m\left(\mathbf{r}\right)$ and $V(\mathbf{r})$ are the local perturbations of the mass (gap) and the chemical potential. A local mass perturbation can be induced by defects in a graphene film or in the substrate [7]. We consider here the delta function model of the perturbation:

$$\delta m\left(\mathbf{r}\right) = -b\delta(r - r_0),\ V(\mathbf{r}) = -a\delta(r - r_0), \tag{2}$$

where r and r_0 are respectively the polar coordinate radius and the perturbation radius. Such short-range perturbation was used in the (3+1)-Dirac problem for narrow-gap and zero-gap semiconductors in [8]. The perturbation matrix elements

$$diag(V_1, V_2)\delta(r - r_0) \tag{3}$$

are related to the a, b parameters as follows

$$-V_1 = a + b,\ \ -V_2 = a - b \tag{4}$$

The delta function perturbation is the simplest solvable short-range model. Finite radius r_0 plays a role of the regulator and is necessary in order to exclude deep states of the atomic energy scale. The finite perturbation radius r_0 leads to the quasi-momentum space form-factor proportional to the Bessel function that justifies our neglect of transitions between the Brillouin band points K and K' [8].

Let us present the two-component spinor in the form

$$\psi_j(\mathbf{r},t)=\frac{\exp\left(-iEt\right)}{\sqrt{r}}\begin{pmatrix} f_j\left(r\right)\exp\left[i\left(j-1/2\right)\varphi\right] \\ g_j\left(r\right)\exp\left[i\left(j+1/2\right)\varphi\right]\end{pmatrix}, \tag{5}$$

where j is the pseudospin quantum number; $j=\pm1/2,\pm3/2,\ldots$. In opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates a degeneracy in the biconic Dirac point. The upper $f_j\left(r\right)$ and lower $g_j\left(r\right)$ components of the spinor satisfy the equations set

$$\frac{dg_j}{dr}+\frac{j}{r}g_j-\left(E-m\right)f_j=\left(a+b\right)\delta(r-r_0)f_j, \tag{6}$$

$$-\frac{df_j}{dr}+\frac{j}{r}f_j-\left(E+m\right)g_j=\left(a-b\right)\delta(r-r_0)g_j. \tag{7}$$

These equations have a symmetry:

$$f_j\leftrightarrow g_j,\ E\rightarrow-E,\ j\rightarrow-j,\ a\rightarrow-a. \tag{8}$$

Let us introduce the function $\varphi_j\left(r\right)\equiv f_j/g_j$. It satisfies the equation:

$$1/\left[\left(a+b\right)\varphi_j^2+\left(a-b\right)\right]\left[\frac{d\varphi_j}{dr}-\frac{2j}{r}\varphi_j-E\left(\varphi_j^2+1\right)\right]+\delta(r-r_0)=0 \tag{9}$$

Integrating in the vicinity of $r=r_0$

$$\lim_{\delta\rightarrow0}\int_{\varphi_j(r_0-\delta)}^{\varphi_j(r_0+\delta)}\frac{d\varphi_j}{\left(a+b\right)\varphi_j^2+\left(a-b\right)}=-1, \tag{10}$$

we obtain the matching condition

$$\arctan\left(\varphi_j^-\sqrt{\left(a+b\right)/\left(a-b\right)}\right)-\arctan\left(\varphi_j^+\sqrt{\left(a+b\right)/\left(a-b\right)}\right)=\sqrt{a^2-b^2},\quad a^2>b^2, \tag{11}$$

where $\varphi_j^-\equiv\varphi_j\left(r_0-\delta\right)$, $\varphi_j^+\equiv\varphi_j\left(r_0+\delta\right)$, $\delta\longrightarrow0$. Excluding the spinor component g_j from the equation set Eq. (6), Eq. (7) in the domains $0\leq r<r_0$ and $r>r_0$, we obtain the second-order equation:

$$\frac{d^2f_j}{dr^2}+\left[E^2-m^2-\frac{j\left(j-1\right)}{r^2}\right]f_j=0. \tag{12}$$

This equation is related to the Bessel one. We assume E to be real and satisfying the inequality $E^2\geq m^2$. Then the general solution of Eq. (12) in the region $0\leq r<r_0$ reads

$$f_j=C_1\sqrt{\kappa r}J_{j-1/2}\left(\kappa r\right)+C_2\sqrt{\kappa r}N_{j-1/2}\left(\kappa r\right), \tag{13}$$

where $\kappa=\sqrt{E^2-m^2}$ is the principal value of the root; $J_\nu\left(z\right)$ and $N_\nu\left(z\right)$ are respectively the Bessel and Neumann functions. The constant C_2 vanishes in the domain $0\leq r<r_0$ since the solution must be regular at the origin.Expressing the g_j-component from Eq. (7), we can write

$$g_j=\sqrt{\frac{E-m}{E+m}}\sqrt{\kappa r}C_1J_{j+1/2}\left(\kappa r\right).$$

Thus

$$\varphi_j^-\left(\kappa r_0\right)=\sqrt{\frac{E+m}{E-m}}\frac{J_{j-1/2}\left(\kappa r_0\right)}{J_{j+1/2}\left(\kappa r_0\right)}. \tag{14}$$

Then we can obtain from Eq. (11):

$$\arctan\left(\sqrt{\frac{a+b}{a-b}}\varphi_j^+\left(\kappa r_0\right)\right)=\arctan\left(\sqrt{\frac{a+b}{a-b}}\sqrt{\frac{E+m}{E-m}}\frac{J_{j-1/2}\left(\kappa r_0\right)}{J_{j+1/2}\left(\kappa r_0\right)}\right)-\sqrt{a^2-b^2}, \tag{15}$$

and, therefore,

$$\varphi_j^+\left(\kappa r_0\right)=\frac{\sqrt{\frac{E+m}{E-m}}J_{j-1/2}\left(\kappa r_0\right)-\left(a-b\right)T\left(a,b\right)J_{j+1/2}\left(\kappa r_0\right)}{J_{j+1/2}\left(\kappa r_0\right)+\left(a+b\right)\sqrt{\frac{E+m}{E-m}}T\left(a,b\right)J_{j-1/2}\left(\kappa r_0\right)}, \tag{16}$$

where $T\left(a,b\right)$ is given by the formula:

$$T\left(a,b\right)=\begin{cases}\frac{\tan\left(\sqrt{a^2-b^2}\right)}{\sqrt{a^2-b^2}} & \text{if } a^2>b^2,\\ \\ \frac{\tanh\left(\sqrt{b^2-a^2}\right)}{\sqrt{b^2-a^2}} & \text{if } b^2>a^2,\end{cases}. \tag{17}$$

On the other hand, an expression for $\varphi_j^+\left(\kappa r_0\right)$ can be written similarly to 14:

$$\varphi_j^+\left(\kappa r_0\right)=\frac{f_j^+}{g_j^+}=\sqrt{\frac{E+m}{E-m}}\frac{H_{j-1/2}^{(2)}\left(\kappa r_0\right)+S_jH_{j-1/2}^{(1)}\left(\kappa r_0\right)}{H_{j+1/2}^{(2)}\left(\kappa r_0\right)+S_jH_{j+1/2}^{(1)}\left(\kappa r_0\right)}, \tag{18}$$

where $S_j\left(\kappa\right)$ is a phase factor of the out-going wave, i. e. S-matrix element in the angular momentum representation. Substituting Eq. (18) into Eq. (16), we obtain an explicit expression for $S_j\left(E\right)$:

$$S_j\left(E\right)=-\frac{\mathcal{F}_j^{(2)}}{\mathcal{F}_j^{(1)}}, \tag{19}$$

where

$$\begin{aligned}\mathcal{F}_j^{(\alpha)} &= \left(J_{j-1/2}\left(\kappa r_0\right)H_{j+1/2}^{(\alpha)}\left(\kappa r_0\right)-J_{j+1/2}\left(\kappa r_0\right)H_{j-1/2}^{(\alpha)}\left(\kappa r_0\right)\right)-\\ &T\left(a,b\right)\left[\sqrt{\frac{E-m}{E+m}}\left(a-b\right)J_{j+1/2}\left(\kappa r_0\right)H_{j+1/2}^{(\alpha)}\left(\kappa r_0\right)+\sqrt{\frac{E+m}{E-m}}\left(a+b\right)J_{j-1/2}\left(\kappa r_0\right)H_{j-1/2}^{(\alpha)}\left(\kappa r_0\right)\right].\end{aligned} \tag{20}$$

Here α takes values $0,1$. Since $H_n^{(2)}\left(z\right)=H_n^{(1)*}\left(z\right)$ for real z, the scattering matrix is unitary everywhere on the continuum spectrum. Eq. (19) solves the electron scattering problem for the given potential. The denominator of $S_j(E)$ is just the left-hand side of the characteristic equation derived in [6]. Imaginary roots of it correspond to the real energy eigenstates (bound states) lying in thegap, which were studied in that paper. The characteristic equation reads

$$\mathcal{F}_j^{(1)}\left(\kappa r_0\right)=0, \tag{21}$$

or

$$\begin{aligned}&\left(J_{j-1/2}\left(\kappa r_0\right)H_{j+1/2}^{(\alpha)}\left(\kappa r_0\right)-J_{j+1/2}\left(\kappa r_0\right)H_{j-1/2}^{(\alpha)}\left(\kappa r_0\right)\right)\\ =\ &T\left(a,b\right)\left[\sqrt{\frac{E-m}{E+m}}\left(a-b\right)J_{j+1/2}\left(\kappa r_0\right)H_{j+1/2}^{(\alpha)}\left(\kappa r_0\right)+\sqrt{\frac{E+m}{E-m}}\left(a+b\right)J_{j-1/2}\left(\kappa r_0\right)H_{j-1/2}^{(\alpha)}\left(\kappa r_0\right)\right]\end{aligned} \tag{22}$$

Using the relations $H_n^{(1)}\left(z\right)=J_n+iN_n$, $H_n^{(2)}=J_n-iN_n$, we can write S-matrix in the form:

$$S_j\left(E\right)=-\frac{A_j\left(E\right)+iB_j\left(E\right)}{A_j\left(E\right)-iB_j\left(E\right)}=\frac{B_j\left(E\right)+iA_j\left(E\right)}{B_j\left(E\right)-iA_j\left(E\right)}, \tag{23}$$

and, therefore, it can be presented in the standard form [10]

$$S_j(E) = \exp\left[i2\delta_j(E)\right], \tag{24}$$

where the scattering phase is given by the expression

$$\delta_j(E) = \arctan\frac{A_j(E)}{B_j(E)}. \tag{25}$$

Formulae (23), (24) show that the scattering matrix $S_j(E)$ is unitary on the continuum spectrum. The functions $A_j(E)$ and $B_j(E)$ are determined as follows

$$A_j(E) = -T(a,b)\left[(a+b)\sqrt{\frac{E+m}{E-m}}J^2_{j-1/2}(\kappa r_0) + (a-b)\sqrt{\frac{E-m}{E+m}}J^2_{j+1/2}(\kappa r_0)\right], \tag{26}$$

$$\begin{aligned} B_j(E) \;=\; & T(a,b)\left[(a+b)\left(\sqrt{\frac{E+m}{E-m}}\right)J_{j-1/2}(\kappa r_0)N_{j-1/2}(\kappa r_0) + (a-b)\sqrt{\frac{E-m}{E+m}}J_{j+1/2}(\kappa r_0)N_{j+1/2}(\kappa r_0)\right] + \\ & \left[J_{j+1/2}(\kappa r_0)N_{j-1/2}(\kappa r_0) - J_{j-1/2}(\kappa r_0)N_{j+1/2}(\kappa r_0)\right] \end{aligned} \tag{27}$$

It is seen from (25), (27) that all $\delta_j(E)$ vanish , when a and b tend to zero, i. e. in the absence of a perturbation. Using the Bessel functions expansion [9]

$$J_n(x) \sim (1/n!)(x/2)^n, \tag{28}$$

$$N_n(x) \sim \begin{cases} -(\Gamma(n)/\pi)(2/x)^n & \text{for } n>0, \\ (2/\pi)\log(\gamma_E x/2) & \text{for } n=0 \end{cases} \tag{29}$$

we conclude that for the low-energy scattering $\kappa r_0 << 1$, $\delta_j(E)$ is small as $(\kappa r_0)^{|j|+1/2}$ except of $j = \pm 1/2$. Here $\log\gamma_E$ is the Eyler-Mascheroni constant. In the case of small radius r_0 and low energy E we can neglect all higher angular momentum partial waves taking into account only phases δ_j for $j = \pm 1/2$:

$$\tan\delta_{1/2}(E) =$$

$$= -T(a,b)\frac{(a+b)\sqrt{\frac{E+m}{E-m}} + (a-b)\sqrt{\frac{E-m}{E+m}}(\kappa r_0/2)^2}{\left[(\kappa r_0/2)\frac{2}{\pi}\log(\gamma_E\kappa r_0/2) - \frac{1}{\pi}(2/\kappa r_0)\right] + T(a,b)\left[(a+b)\sqrt{\frac{E+m}{E-m}}\frac{2}{\pi}\log(\gamma_E\kappa r_0/2) + (a-b)\sqrt{\frac{E-m}{E+m}}\frac{\Gamma(1)}{\pi}\right]} \approx$$

$$T(a,b)\sqrt{\frac{E+m}{E-m}}(a+b)\,\pi\left(\frac{\kappa r_0}{2}\right),\ \kappa r_0 \longrightarrow 0 \tag{30}$$

$$\tan\delta_{-1/2}(E) =$$

$$= -T(a,b)\frac{(a-b)\sqrt{\frac{E-m}{E+m}} + (a+b)\sqrt{\frac{E+m}{E-m}}(\varkappa r_0/2)^2}{\left[\frac{\Gamma(1)}{\pi}(2/\kappa r_0) - (\kappa r_0/2)\frac{2}{\pi}\log(\gamma_E\kappa r_0/2)\right] + T(a,b)\left[\sqrt{\frac{E-m}{E+m}}(a-b)\frac{2}{\pi}\log(\gamma_E\kappa r_0/2) + \sqrt{\frac{E+m}{E-m}}(a+b)\frac{\Gamma(1)}{\pi}\right]} \approx$$

$$-T(a,b)\sqrt{\frac{E-m}{E+m}}(a-b)\,\pi\left(\frac{\kappa r_0}{2}\right), \quad \kappa r_0 \longrightarrow 0 \tag{31}$$

We see that the phase is proportional to κr_0 in the long-wave limit as it is necessary [10], [4]. The scattering amplitude $f(\theta)$ and transport cross-section Σ_{tr} can be expressed in terms of $S_j(E)$ as follow [4]:

$$f(\theta) = \frac{1}{i\sqrt{2\pi\kappa}} \sum_{j=\pm 1/2, \pm 3/2, \ldots} \left[S_j(E) - 1\right] \exp\left[i\left(j - 1/2\right)\theta\right], \tag{32}$$

$$\Sigma_{tr} = 2/\kappa \sum_{j=\pm 1/2, \pm 3/2, ..} \sin^2\left(\delta_{j+1} - \delta_j\right) \tag{33}$$

Near the resonance states the Breit-Wigner form of the phase is valid [10]:

$$\delta_j \approx \delta_j^{(0)} + \arctan \frac{\Gamma_j}{2\left(E_j^{(0)} - E\right)},$$

where $E_j^{(0)}$ and Γ_j are respectively the position and width of the resonance level, $\delta_j^{(0)}$ is the slowly-varying potential scattering phase.

The presented above formulae can be used in order to calculate the Boltzmann conductivity [11]

$$\sigma = \left(\frac{e^2}{2\pi\hbar}\right) \frac{2E_F}{\hbar} \tau_{tr}, \tag{34}$$

where the transport relaxation time equals

$$1/\tau_{tr} = N_i v_F \Sigma_{tr}. \tag{35}$$

Here N_i is the areal impurity density, $E_F = v_F \kappa_F$. The above equations transform a dependence of the scattering data on the Fermi energy and impurity perturbation parameters a and b into the correspondent dependence of the Boltzmann conductivity. Thus characteristic features of the scattering data determine a behaviour of the electric conductivity. Proper numeric calculations will be presented elsewhere.

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